Try Anything Once: A Case Study using NUCCOR

Rebecca Hartman-Baker
Scientific Computing Group
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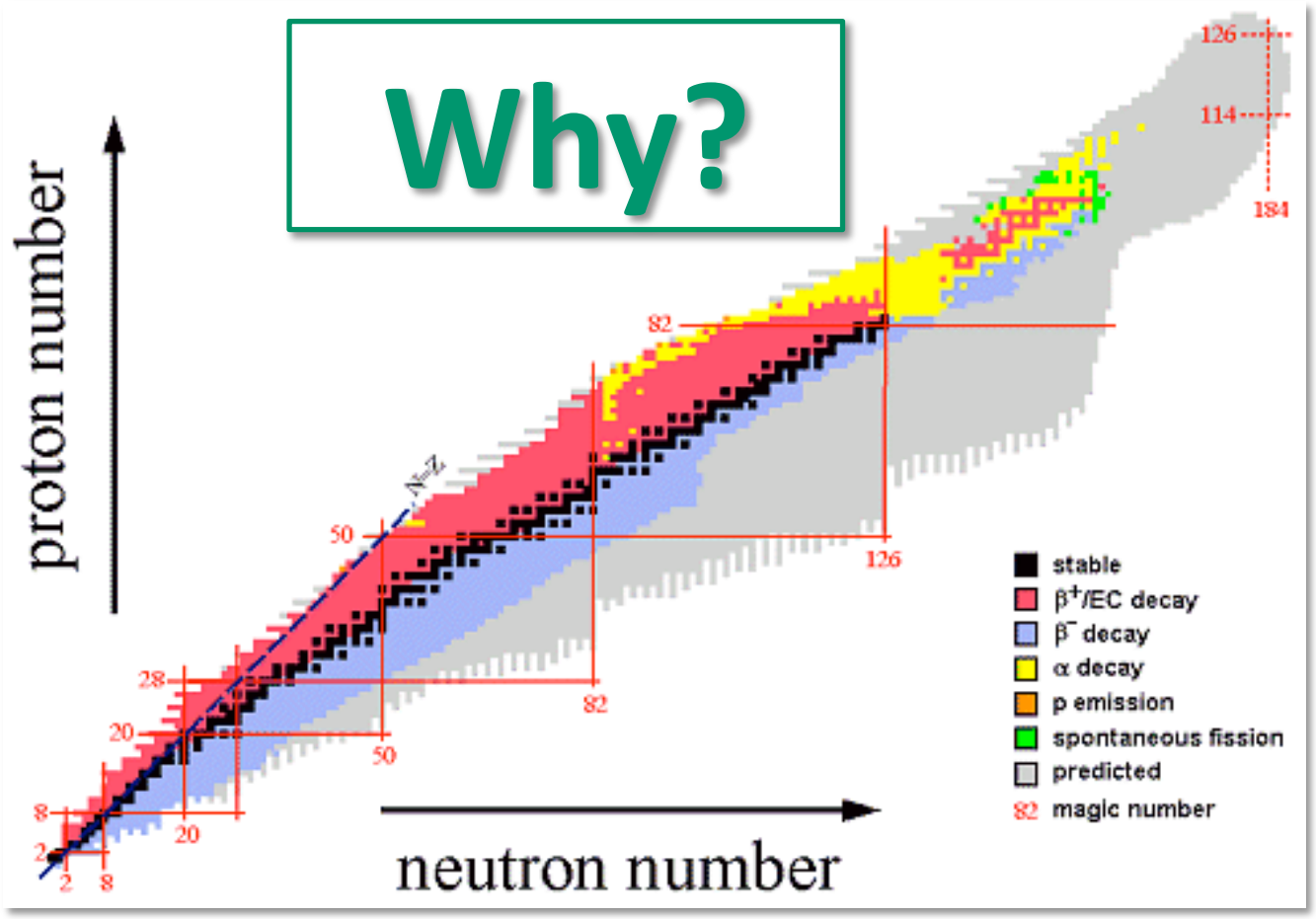
Outline

- Nuclear Physics in 5 slides or less
- Motivation for this work
- Experiments
- Results
- Addendum: Cray compiler and loop optimization
- Conclusions

Nuclear Physics: Basics

- Nucleus consists of protons and neutrons
- Like electrons, protons and neutrons in energy-level shells
- Some configurations more stable than others

Nuclear Physics: Table of Nuclides



Source: http://fys246.nuclear.lu.se/images/nucchrt2.gif

Nuclear Physics: NUCCOR code

- Nuclear Coupled-Cluster Oak Ridge code
- CCSD: approximates interactions between nucleons using single and double excitation states
- Essentially, solving huge set of coupled nonlinear equations
- Written in Fortran 90, with modules, derived datatypes
- Runs are constrained primarily by memory – lots of data, (relatively) low flop count

Motivation: My Job

- Improve code so that it
  - Scales better
  - Runs faster
- My (not-so-)secret techniques
  - Investigate/model performance of existing code
  - Implement better parallel I/O
  - Implement load balancing
  - Clean up wasteful/bad coding practices
  - Help code adhere to Fortran standards

Motivation: Events

- Grad student's version of code segfaulted only with Intel compiler, only with optimizations turned on, only on Jaguar
  - First guess: seat-to-keyboard interface problem
  - Turned out to be compiler bug!
- Talked to nuclear physicists
  - Depend heavily on Intel compiler
  - Reluctant to take risks with code
- I'm free to take risks and optimize code – I'm in this for performance, not science!
  - Make sure that optimizations do not result in incorrect answers, but nothing new comes out of my benchmarks

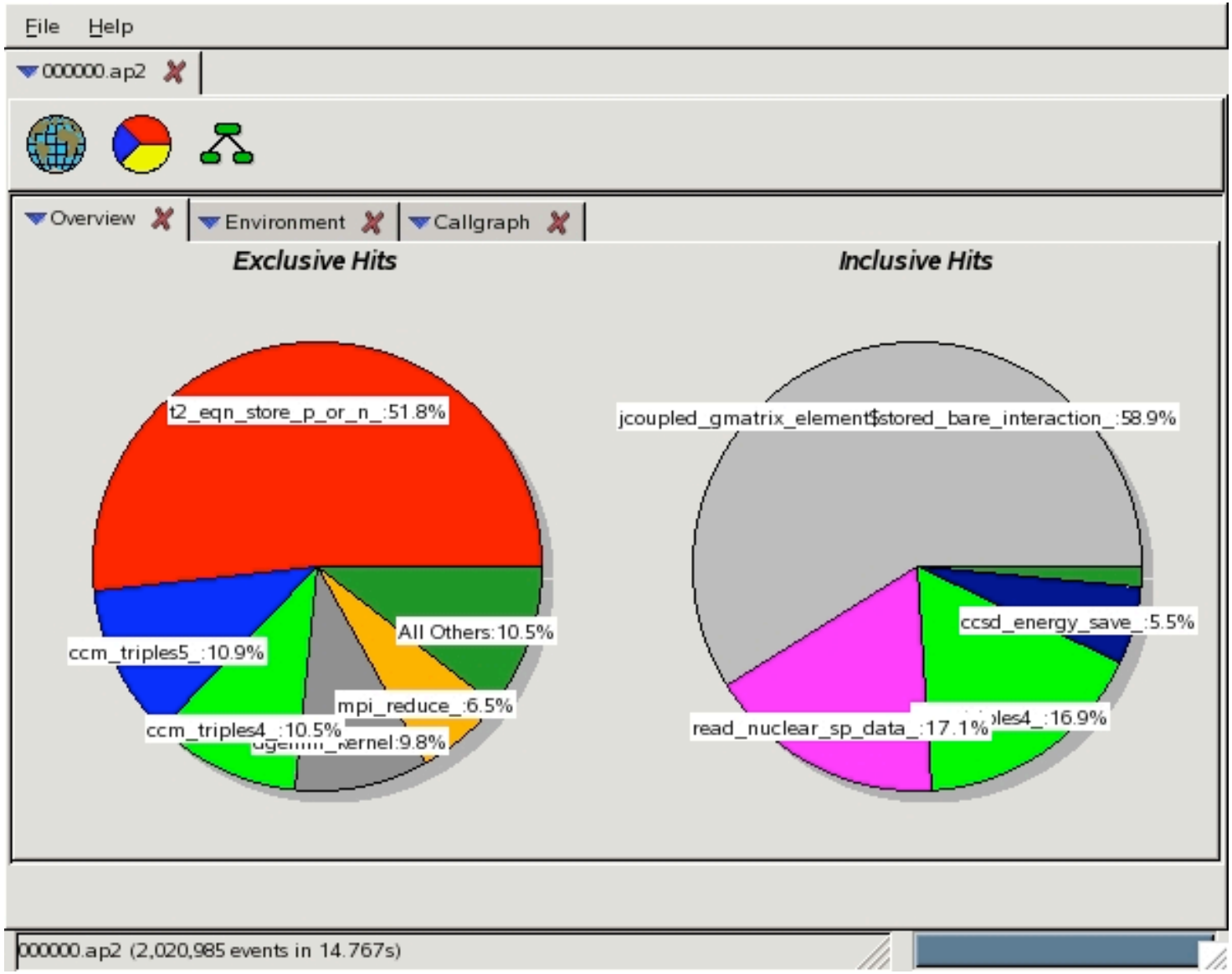
Motivation: Questions

- What is happening in this code?
  - Where is the most time spent?
  - What are the bottlenecks?
- How does the compiler impact performance?
  - Do compiler optimizations really matter?
  - Do different compilers perform differently?

Experiments: Performance

- Instrumented optimized code with Craypat
  - `module load xt-craypat apprentice2`
  - `make clean; make`
  - `pat_build -O apa mycode` (this creates executable called `mycode+pat`)
  - `qsub patscript`
- Generated reports using `pat_report` (this took a while)
- Viewed reports with Apprentice2: `app2 file.ap2` (loading this also took a while)

Craypat Results



Craypat Results

- Most time spent in `t2_eqn_store_p_or_n`
- This function full of deeply nested loops (very ugly)
- Text report provides info on which lines within subroutine take up the most time
- Many different pieces take up small portions of time, but overarching theme is time taken by performing iterative updates

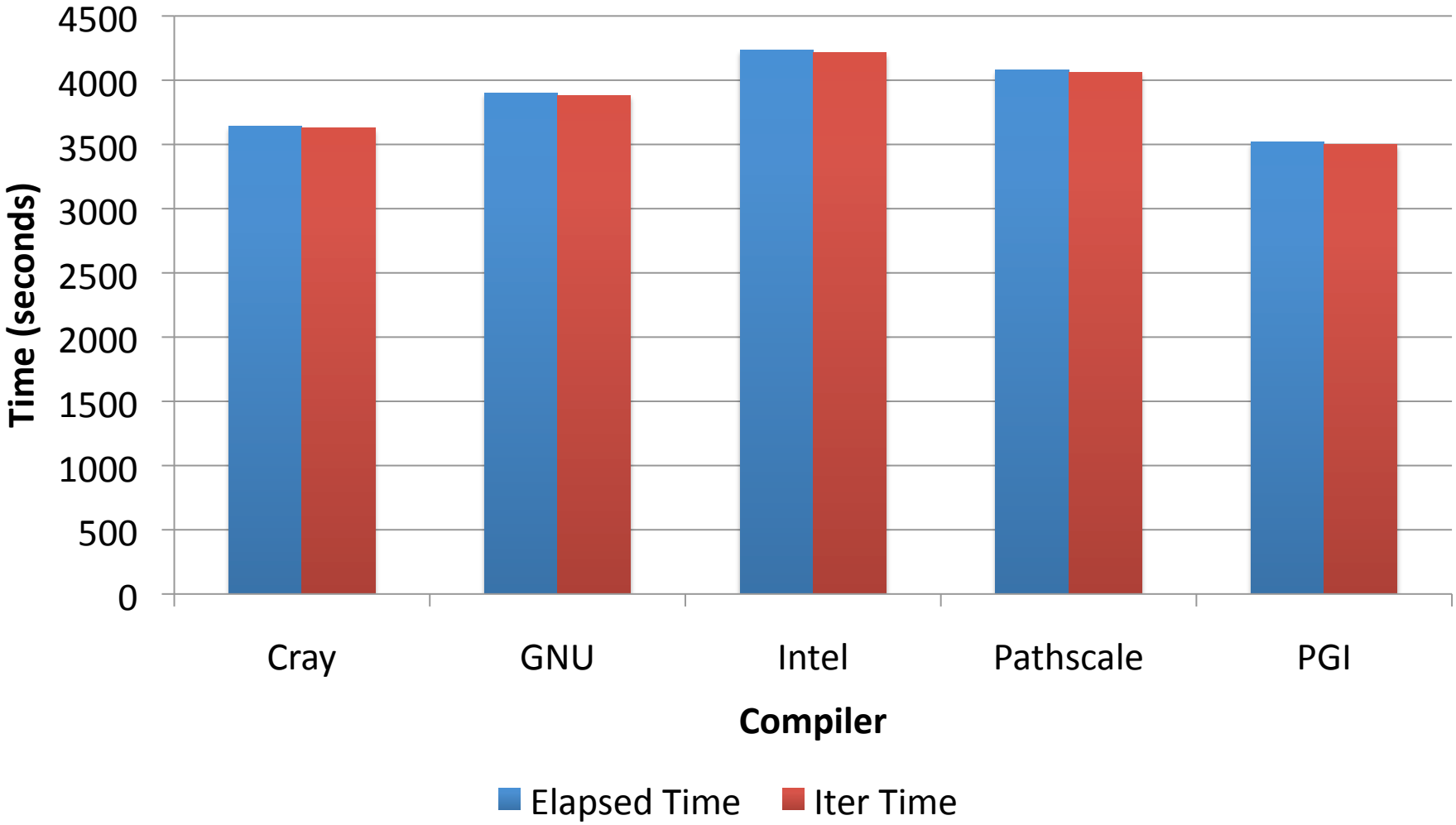
Experiments: Compiler Tests

- Compiled NUCCOR with all 5 compilers available on Jaguar (Cray, GNU, Intel, Pathscale, PGI)
- For each compiler, 6 different optimization levels (-O0, -O1, -O2, -O3, default, high)
- Ran each executable 3 times on ^{16}O benchmark, 441 processors, using 8 cores/node on Jaguarpf:
  - `aprun -n 441 -S4 nuccor.exe`
- Checked that each executable produced correct results (what good is getting the wrong answer quickly?)

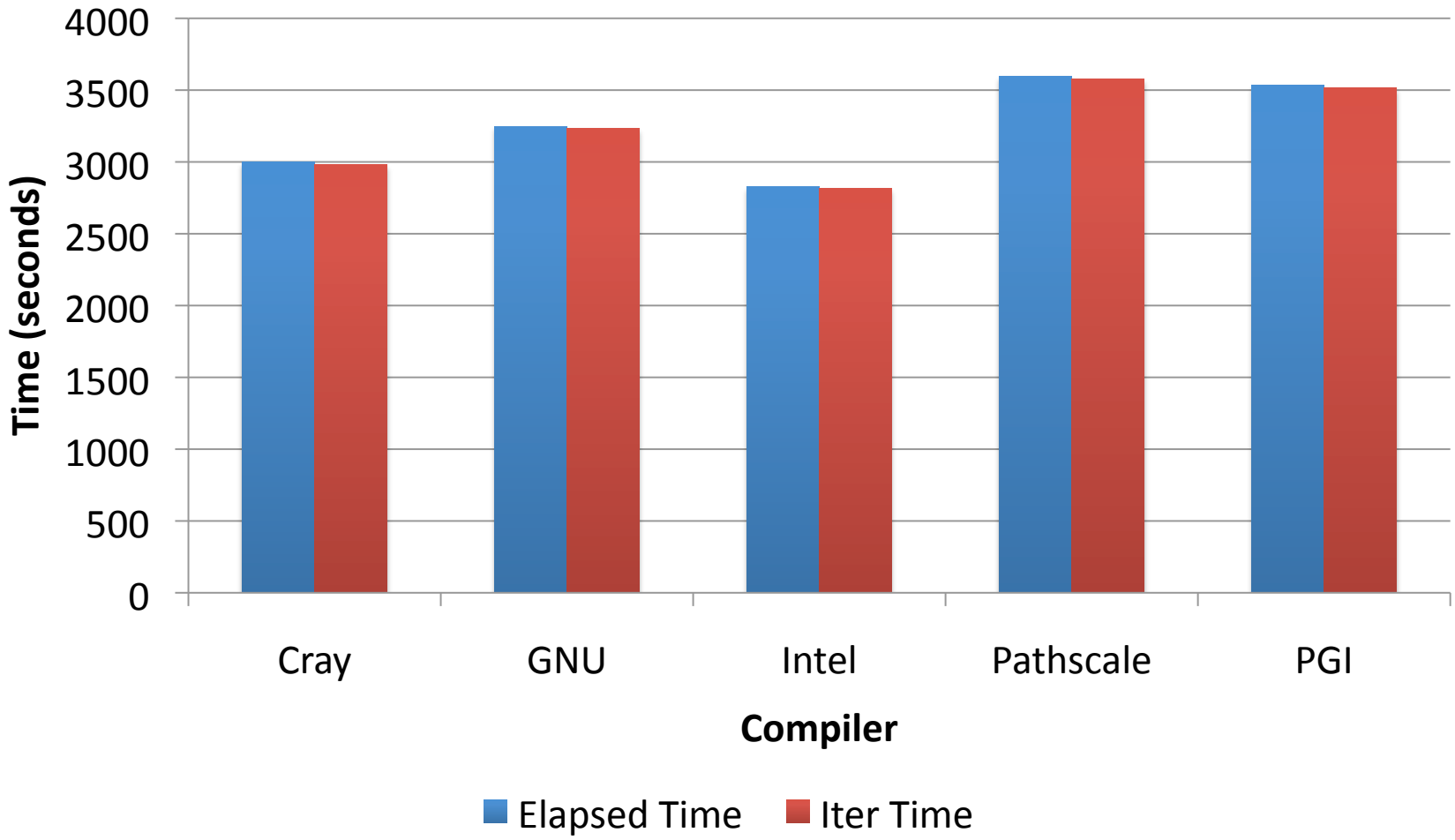
Experiments: Compiler Information

Compiler	Version	High Optimization flags
Cray	7.1.5 (default)	`-O3`
GNU	4.4.2 (default)	`-O2 -ffast-math -fomit-frame-pointer -mfpmath=sse`
Intel	11.1.046 (default)	`-O3`
Pathscale	3.2 (default)	`-Ofast`
PGI	9.0.4 (default)	`-fast`

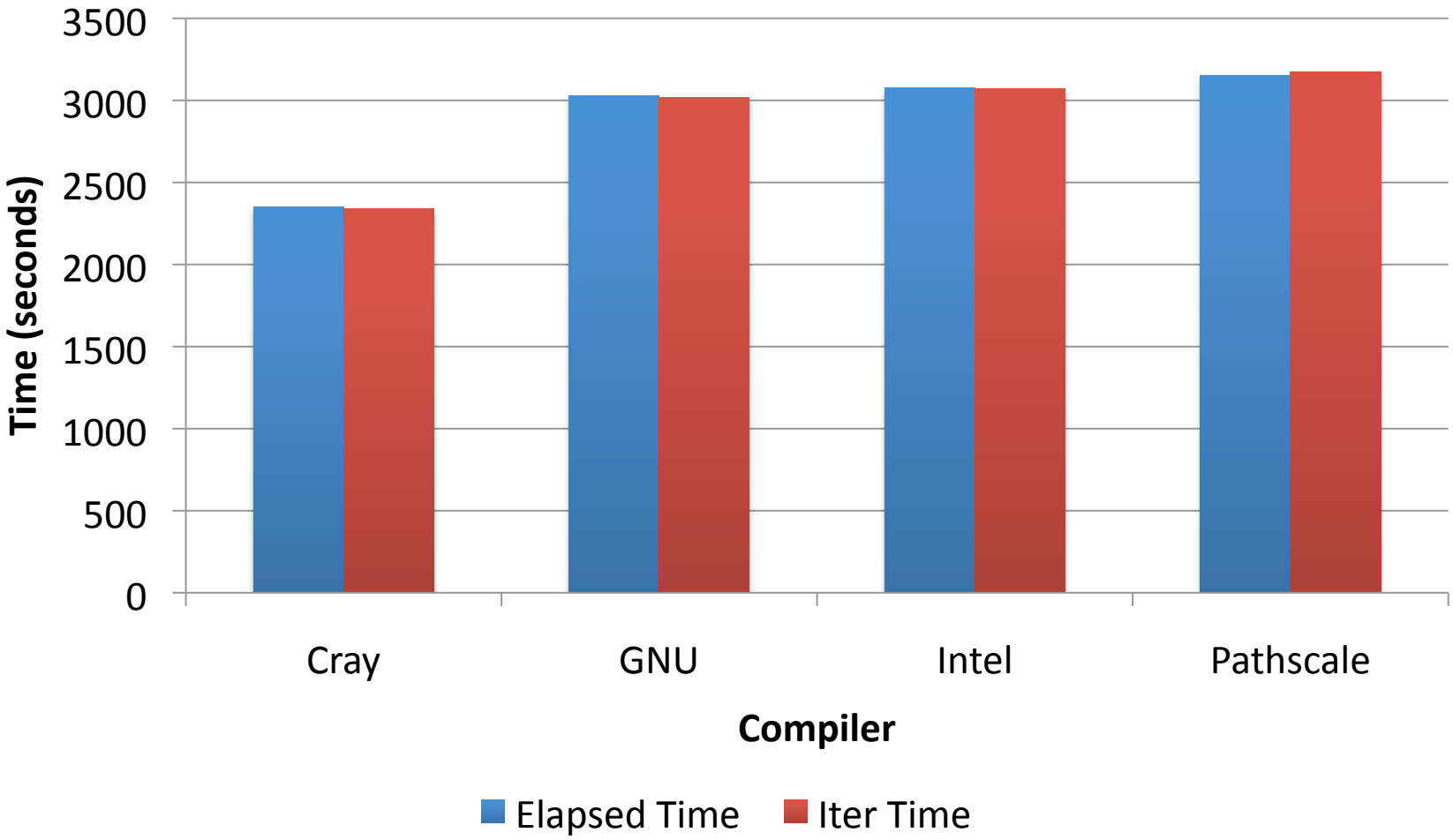
Results: -O0 Optimization Level



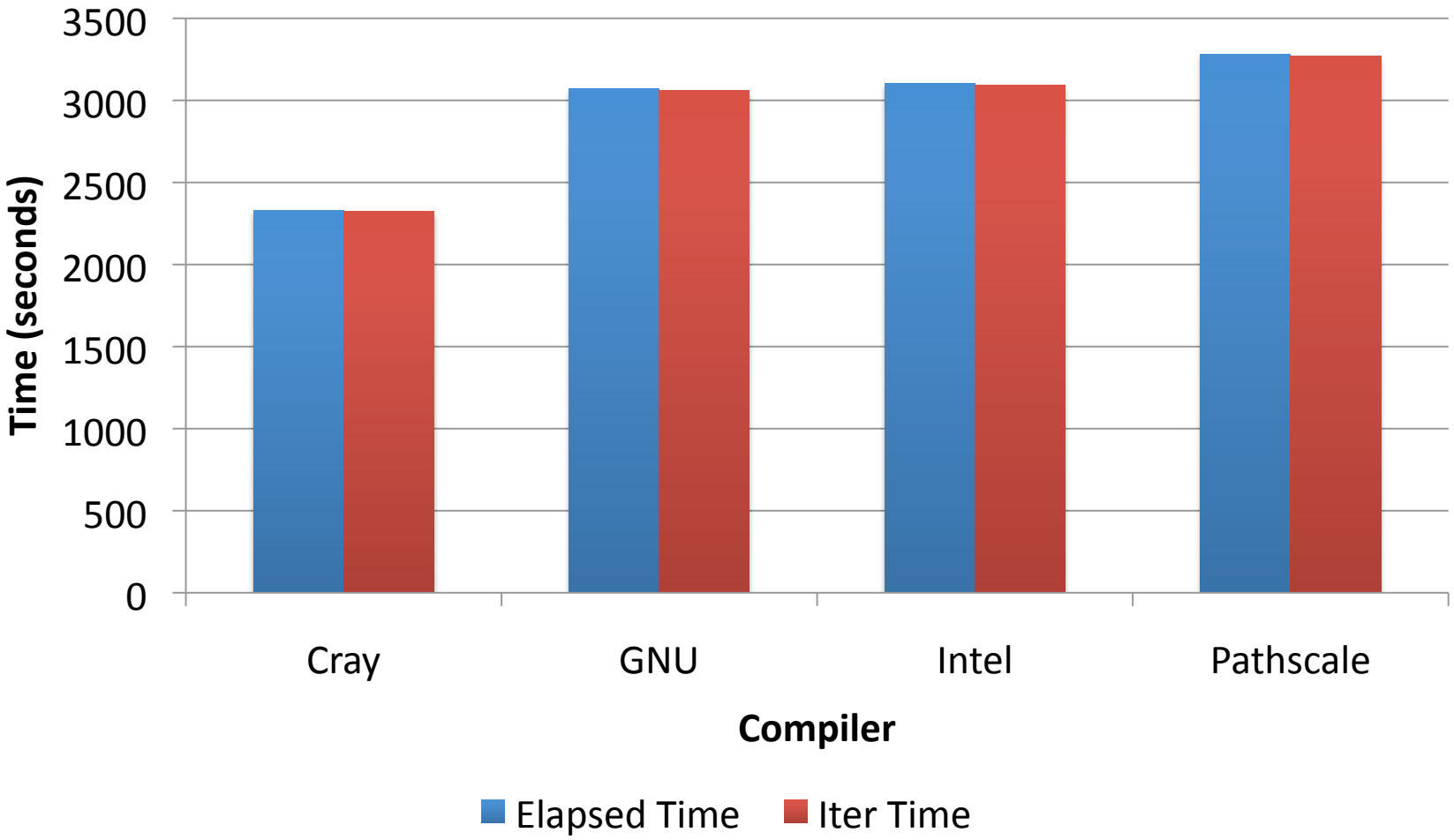
Results: -O1 Optimization Level



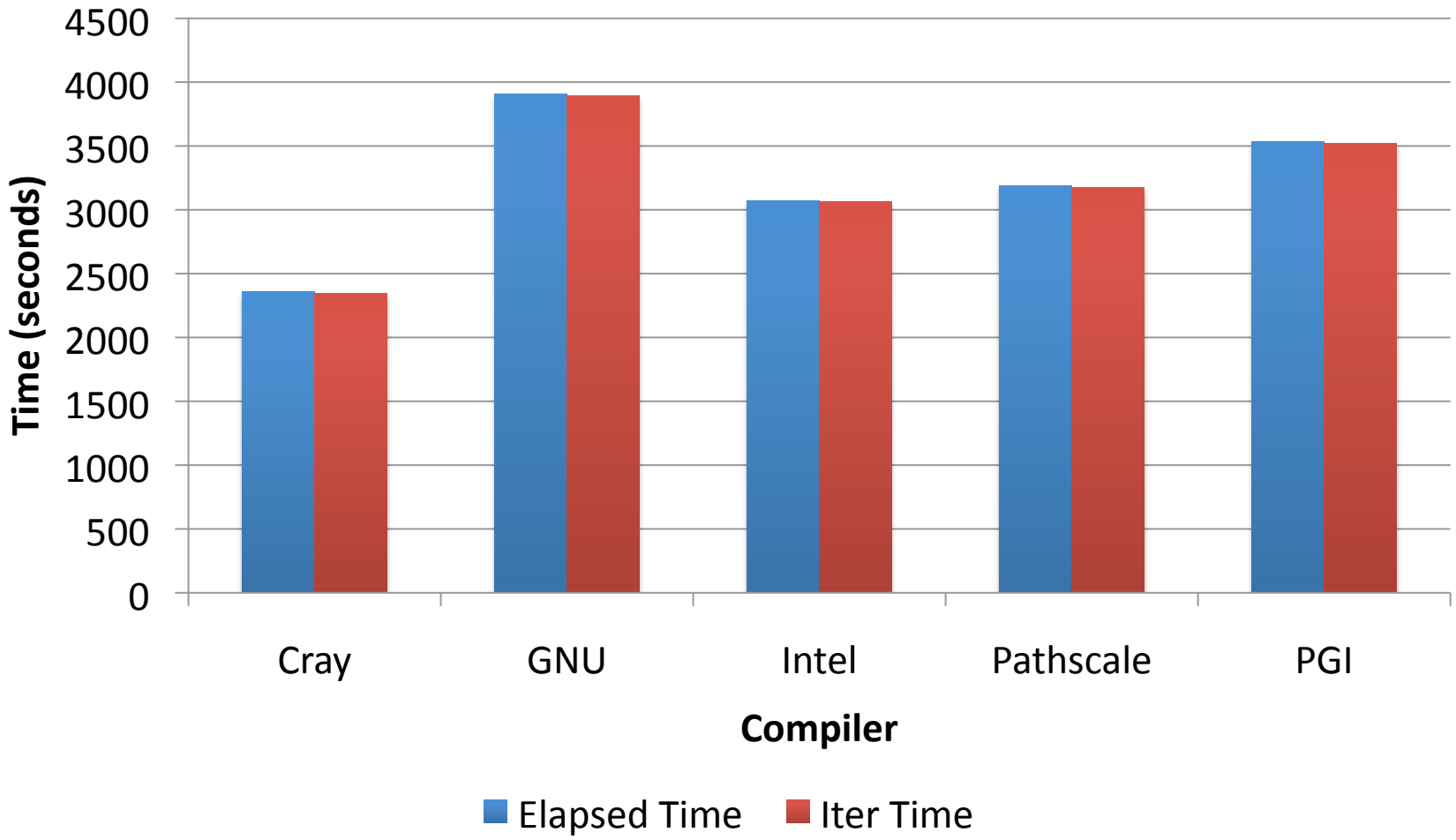
Results: -O2 Optimization Level



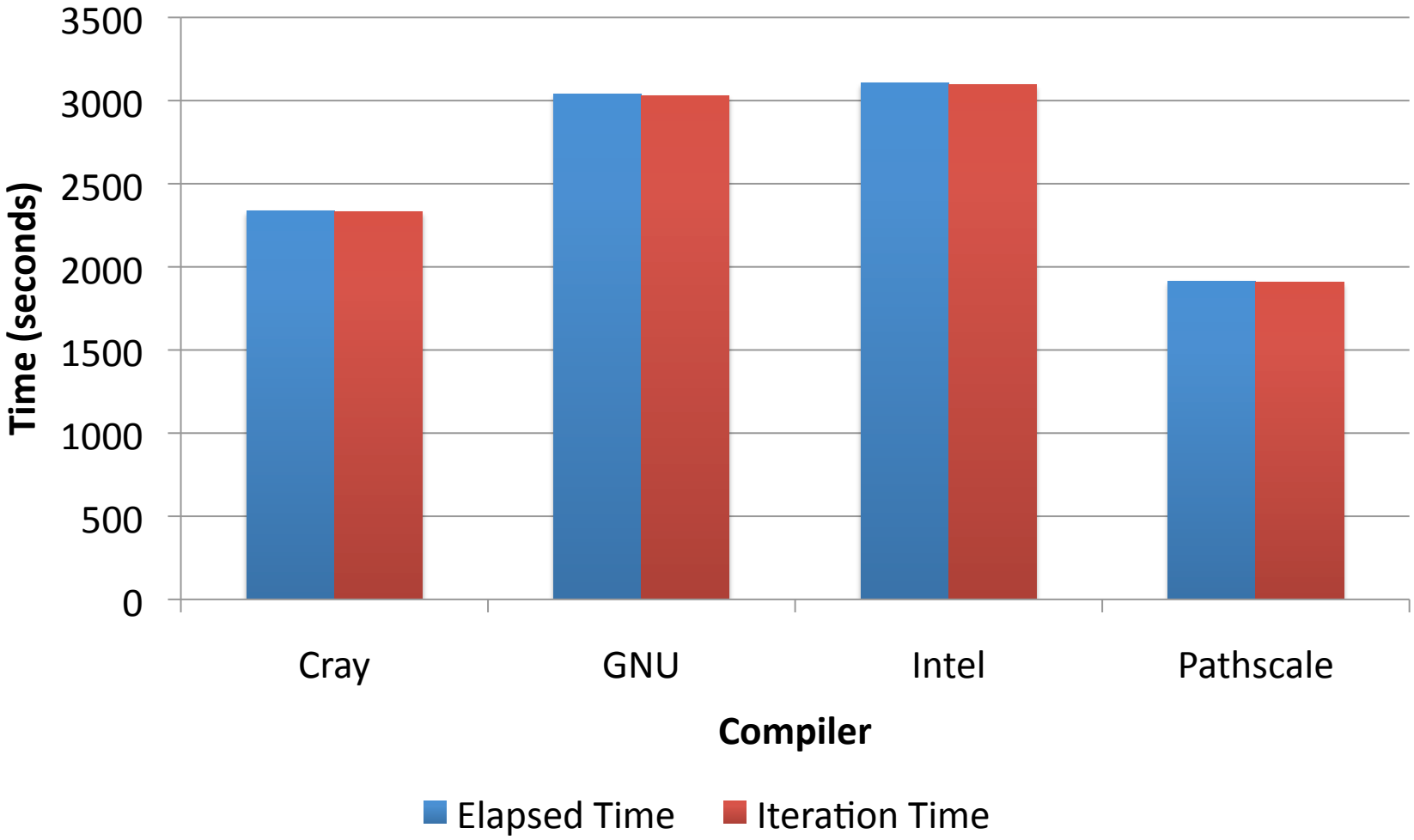
Results: -O3 Optimization Level



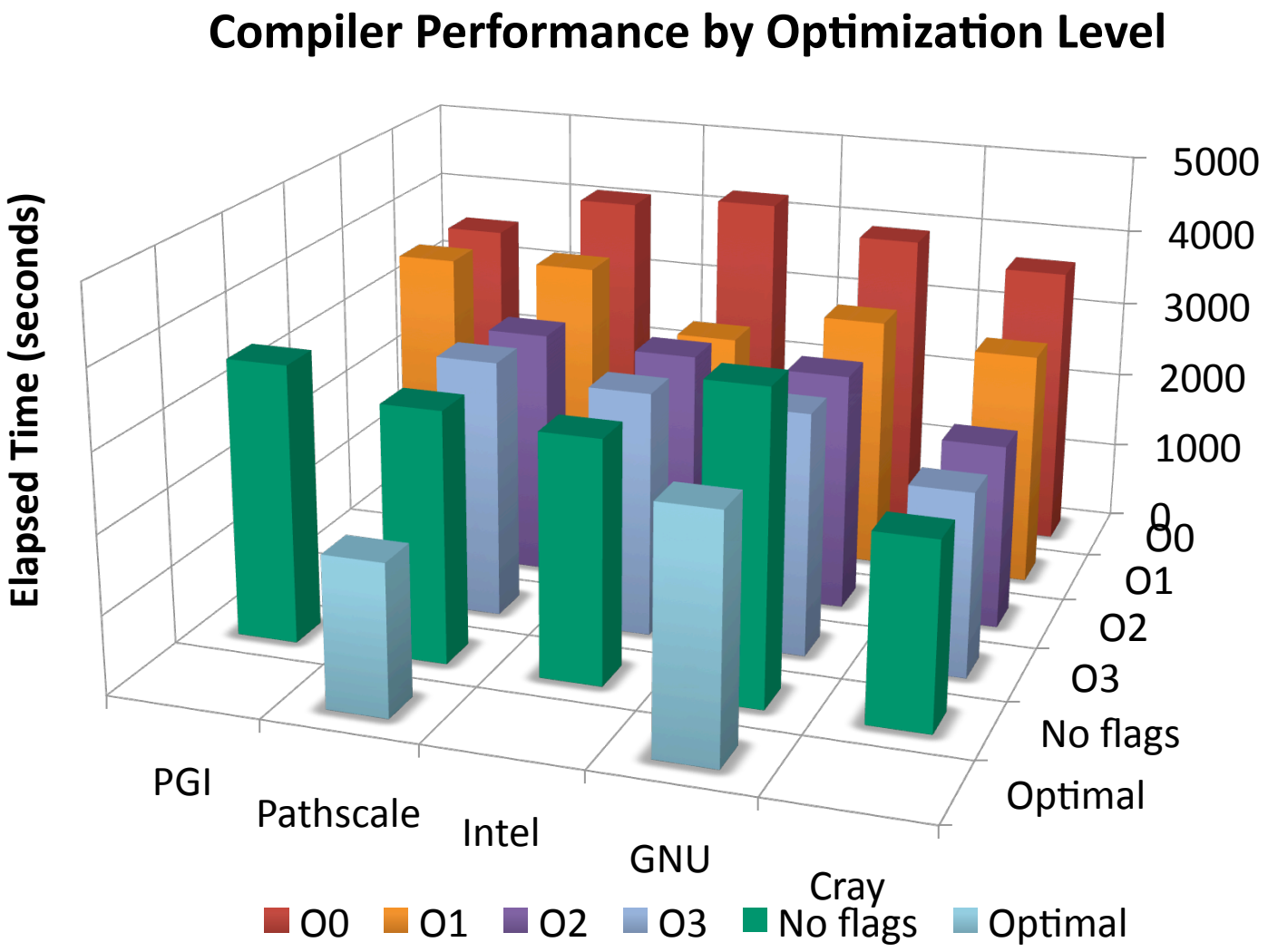
Results: Default Optimization Level



Results: High Optimization Level



Results: Aggregate Performance Results



Results: Best Performance at Each Optimization Level

Optimization Level	Top Performer	2nd Best Performer	% Difference in walltime between 1st and 2nd best performers
-O0	PGI	Cray	3.54
-O1	Intel	Cray	5.88
-O2	Cray	GNU	25.2
-O3	Cray	GNU	27.3
No flags	Cray	Intel	26.4
Optimal	Pathscale	Cray	20.5

Overall winner: Cray compiler!

Addendum: Cray Compiler

- I discussed results with Jeff Larkin, including surprise Pathscale victory
- He suggested sending code to Cray compiler developers, so they can improve their compiler
- Last week I received very nice, very detailed analysis of where Cray compiler did not optimize
  - Cray also opened ticket against this issue, and will fix it in next release
- Lessons can be applied to code and improve performance across all compilers

Addendum: Loop Optimization

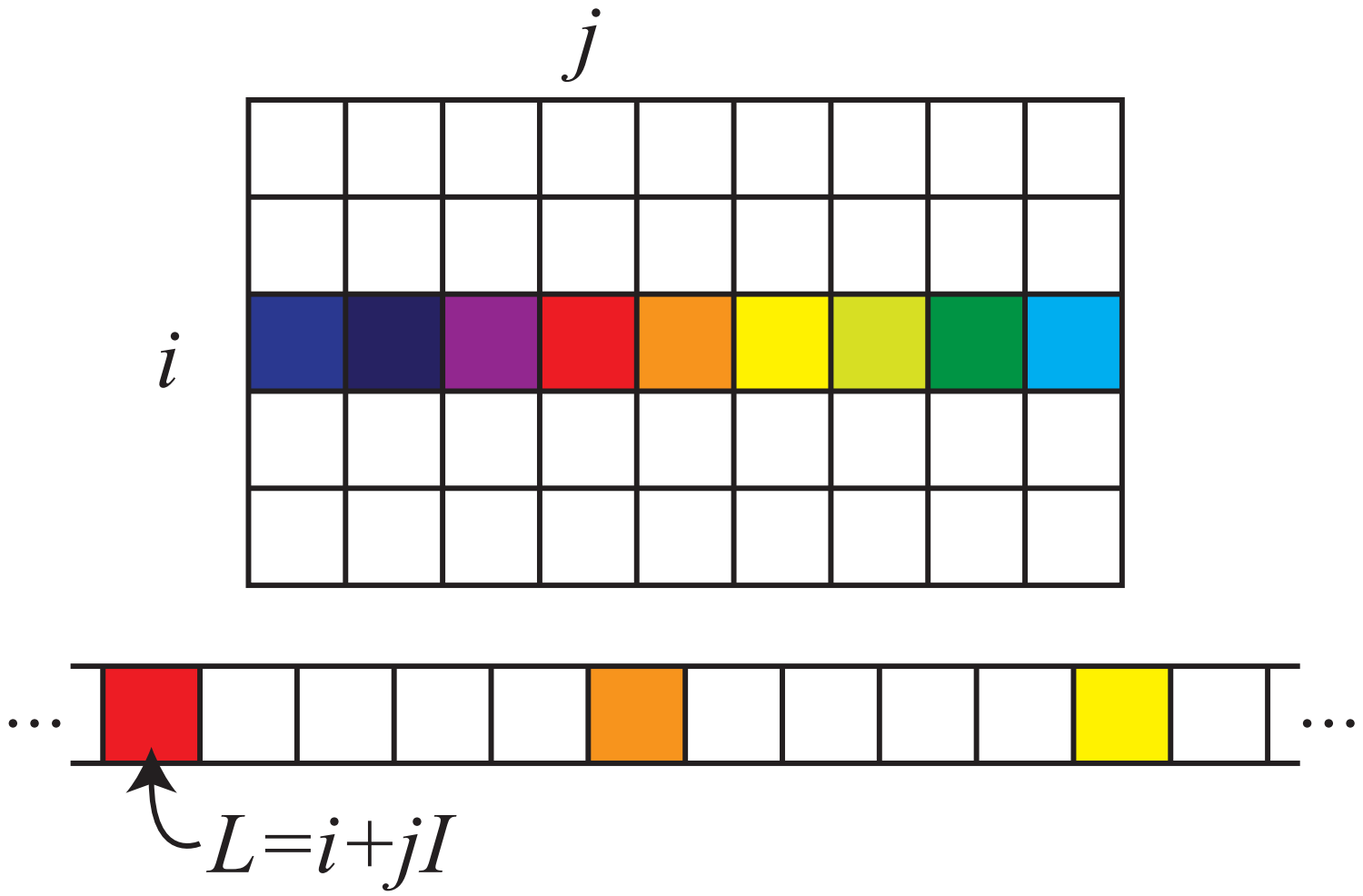
- Nuccor contains many deeply nested loops (depth 4)
- Loops written symmetrically for readability
- But, not easy for compiler to optimize

```
ii=0
do b=below_ef+1,tot_orbs
do j=1,below_ef
  ii=ii+1
  jj=0
  do a=below_ef+1,tot_orbs
  do i=1,below_ef
    jj=jj+1
    t2_ccm_eqn%f5d(a,b,i,j)= t2_ccm_eqn%
        f5d(a,b,i,j) + tmat7(ii,jj)
    t2_ccm_eqn%f5d(b,a,i,j)= t2_ccm_eqn%
        f5d(b,a,i,j) - tmat7(ii,jj)
    t2_ccm_eqn%f5d(a,b,j,i)= t2_ccm_eqn%
        f5d(a,b,j,i) - tmat7(ii,jj)
    t2_ccm_eqn%f5d(b,a,j,i)= t2_ccm_eqn%
        f5d(b,a,j,i) + tmat7(ii,jj)
    ops_cnt=ops_cnt+4
  end do
  end do
end do
end do
```

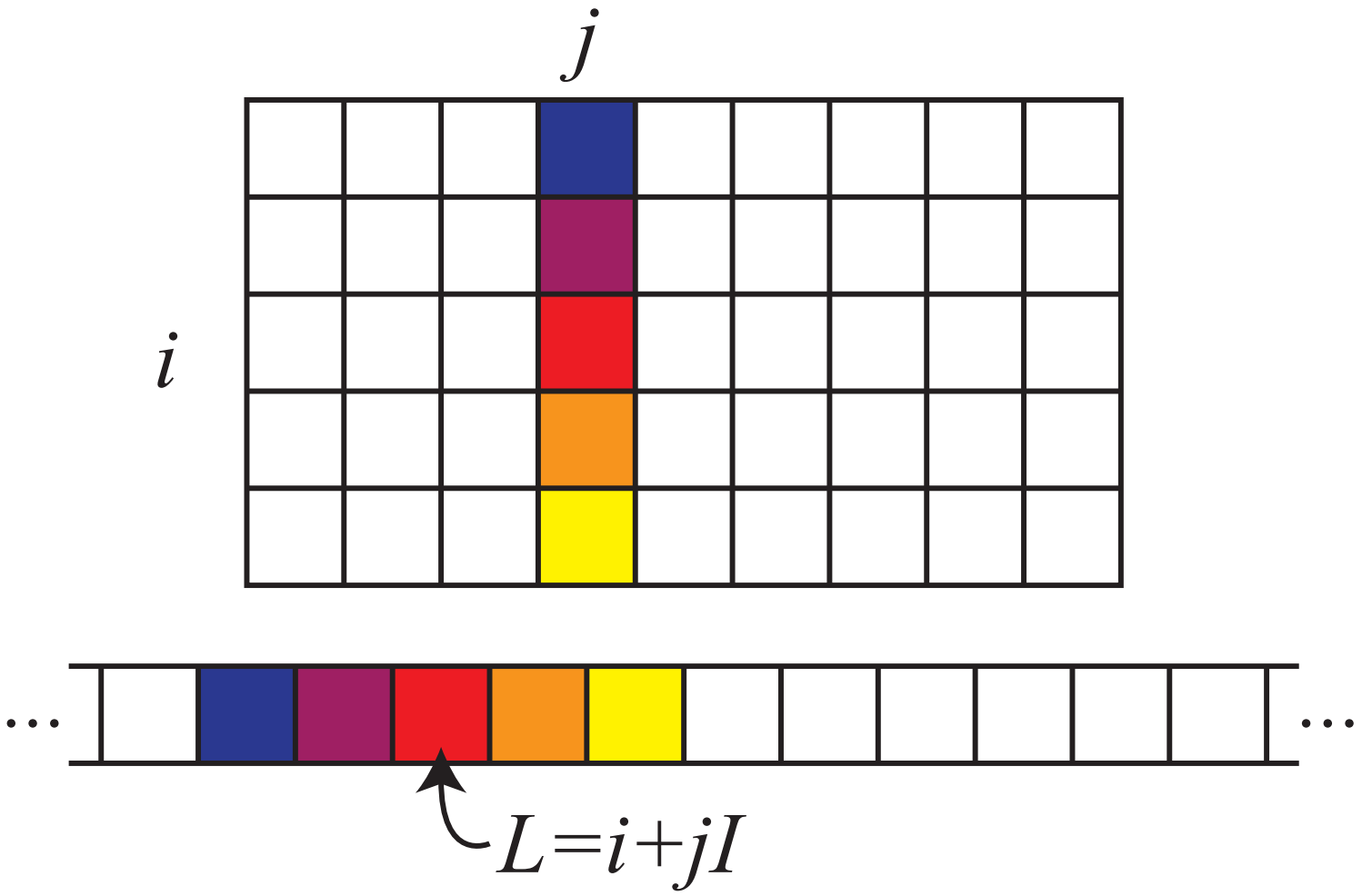
Problems in Loop

- Loop is easy for humans to read
- But, strides through memory cause cache thrashing and increased bandwidth use
- With `below_ef = 16` and `tot_orbs = 336`, each cache line of `t2_ccm_eqn%f5d` will have to be reloaded 8 times
- Also, array `tmat7(ii,jj)` referenced through 2nd subscript, so poor stride
- All compilers (except maybe Pathscale with `-Ofast`) fail to interchange loop nesting

Loop Memory Access (Poor Stride)



Loop Memory Access (Good Stride)



Compiler Optimizations

- Cray compiler will output annotated version of source file
  - `ftn -rm mycode.f90`
  - Outputs `mycode.lst`
- Examine annotated file to figure out what's going on

```
Primary Loop Type          Modifiers
------- ---- ----          ---------
A - Pattern matched        a - vector atomic memory operation
                           b - blocked
C - Collapsed              c - conditional and/or computed
D - Deleted                f - fused
E - Cloned
I - Inlined                i - interchanged
M - Multithreaded          m - partitioned
P - Parallel               p - partial
R - Redundant              r - unrolled
                           s - shortloop
V - Vectorized             t - array syntax temp used
                           w - unwound
```

Annotated Loop

```
371.                    ii=0
372.1--------<          do b=below_ef+1,tot_orbs
373.1 2------<          do j=1,below_ef
374.1 2                   ii=ii+1
375.1 2                   jj=0
376.1 2 3----<            do a=below_ef+1,tot_orbs
377.1 2 3 r8-<            do i=1,below_ef
378.1 2 3 r8                jj=jj+1
379.1 2 3 r8                t2_ccm_eqn%f5d(a,b,i,j)=… +tmat7(ii,jj)
380.1 2 3 r8                t2_ccm_eqn%f5d(b,a,i,j)=… -tmat7(ii,jj)
381.1 2 3 r8                t2_ccm_eqn%f5d(a,b,j,i)=… -tmat7(ii,jj)
382.1 2 3 r8                t2_ccm_eqn%f5d(b,a,j,i)=… +tmat7(ii,jj)
383.1 2 3 r8                ops_cnt=ops_cnt+4
384.1 2 3 r8->            end do
385.1 2 3---->            end do
386.1 2------>          end do
387.1-------->          end do
```

Unroll loop 8 times

Loop Reordering: Two Things to Try

- *Improve stride:* reorder so that `tmat7` is accessed by consecutive row, not column
- *Loop fission:* put all `f5d(a,b,:,:)` in one loop, all `f5d(b,a,:,:)` in another
- Test these two ideas in simple loop unrolling code

Test Code: Original Loop

```
ii = 0
do b = abmin, abmax
   do j = ijmin, ijmax
      ii = ii+1
      jj = 0
      do a = abmin, abmax
         do i = ijmin, ijmax
            jj = jj+1
            f5d(a,b,i,j) = f5d(a,b,i,j) + tmat7(ii,jj)
            f5d(b,a,i,j) = f5d(b,a,i,j) - tmat7(ii,jj)
            f5d(a,b,j,i) = f5d(a,b,j,i) - tmat7(ii,jj)
            f5d(b,a,j,i) = f5d(b,a,j,i) + tmat7(ii,jj)
         end do
      end do
   end do
end do
```

Test Code: Improved Stride

```
do i = ijmin, ijmax
   jj = 0
   do a = abmin, abmax
      do j=ijmin, ijmax
         jj = jj+1
         ii = 0
         do b = abmin, abmax
            ii = ii+1
            f5d(a,b,i,j) = f5d(a,b,i,j) + tmat7(ii,jj)
            f5d(b,a,i,j) = f5d(b,a,i,j) - tmat7(ii,jj)
            f5d(a,b,j,i) = f5d(a,b,j,i) - tmat7(ii,jj)
            f5d(b,a,j,i) = f5d(b,a,j,i) + tmat7(ii,jj)
         end do
      end do
   end do
end do
```

Test Code: Loop Fission

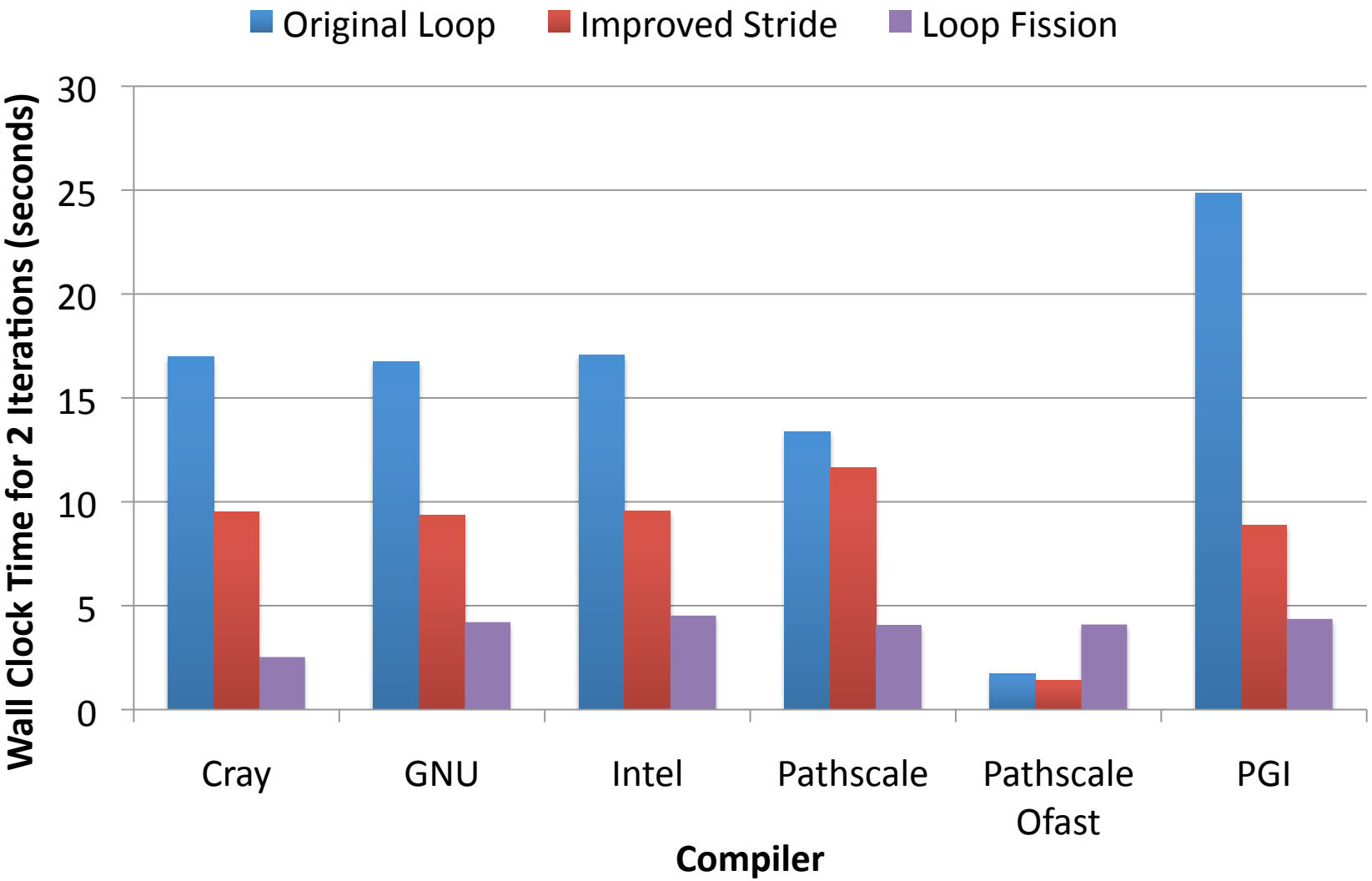
```
ii = 0
do j = ijmin, ijmax
   do b = abmin, abmax
      ii = ii+1
      jj = 0
      do i = ijmin, ijmax
         do a = abmin, abmax
            jj = jj+1
            f5d(a,b,i,j) =
              f5d(a,b,i,j) +
              tmat7(ii,jj)
            f5d(a,b,j,i) =
              f5d(a,b,j,i) -
              tmat7(ii,jj)
         end do
      end do
   end do
end do
```

```
jj = 0
do i = ijmin, ijmax
   do a = abmin, abmax
      jj = jj+1
      ii = 0
      do j = ijmin, ijmax
         do b = abmin, abmax
            ii = ii+1
            f5d(b,a,i,j) =
              f5d(b,a,i,j) -
              tmat7(ii,jj)
            f5d(b,a,j,i) =
              f5d(b,a,i,j) +
              tmat7(ii,jj)
         end do
      end do
   end do
end do
```

Test Code: Cray Compiler Behavior

- Original Loop: unrolled 8 times
- Improved Stride: conditionally vectorized, unrolled 2 times
- Loop Fission: 1st loop vectorized, partially unrolled 4 times; 2nd loop vectorized, unrolled 4 times

Test Code: Performance of All Compilers



Conclusions

- Things I learned from this exercise
  - Some parts of code were not standard Fortran (They are now!)
  - All optimizations produced identical results for this computation
  - Cray compiler is very good with Fortran, as advertised
  - Cray compiler developers very responsive to user feedback
  - Loop ordering makes HUGE difference
  - Try anything once!

Acknowledgments

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